

A REINTRODUCTION OF DYNAMICAL $SU(2)$ GAUGE FIELDS IN HUBBARD MODELS

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Abstract

This is a brief discussion of an old preprint (which follows). This paper explains how non-Abelian gauge magnets originate as effective dynamics in models of hopping particles. In particular, an explicit model is discussed in which both link and plaquette terms appear. The motivation to reintroduce the idea is some recent theoretical progress on the topic of optical lattices.

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An Apology

Recently there have appeared some intriguing results on how dynamical gauge invariance may occur in optical lattices [1]. In particular, it appears that Abelian gauge magnets of the type discussed in [2] could arise. The authors of Reference [1] present a detailed discussion as to how such a model can be simulated. In the light of these developments, it may be timely to reintroduce the paper from 1990, entitled “SU(2) Gauge Invariance in Hubbard Models and Superconductivity”. The main point was that a non-Abelian gauge magnet appears in the hopping-parameter expansion of a particular Hubbard model. The paper has been available only as a scanned manuscript [3] until now.

The paper concerns only dynamical non-Abelian gauge fields. Background non-Abelian gauge fields have been discussed in References [4].

I have not revised the paper except to update the references and to correct a few misprints. The model was proposed to explain copper-oxide-layer superconductivity, through either confinement or screening of spin. Applying the model to optical lattices may be worthy of investigation.

The only other reason for this apology is to mention that there is a very general context in which gauge magnets [5] (also known as “quantum link models”), both Abelian and non-Abelian, should appear at low frequencies. Indeed, there appears to be a general theorem concerning how such models arise in the hopping-parameter expansion. I intend to explain how this theorem works elsewhere.

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SU(2) GAUGE INVARIANCE IN HUBBARD MODELS AND SUPERCONDUCTIVITY

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Abstract

It is suggested that in doped copper oxide layers, the lowest energy p_x oxygen orbital for a hole is split by lattice distortions, into states which hybridize asymmetrically with the $d_{x^2-y^2}$ orbitals on each of the neighboring copper atoms. The appropriate Hubbard model has two available sites associated with each oxygen atom. The system is effectively described by an SU(2) gauge theory, with an additional coupling to a charged spinning superfluid. Spin is thereby either confined or screened. Both possibilities lead to hole pairing and superconductivity.

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1 Introduction

Magnetic, rather than phononic, dynamics is widely believed to be responsible for high temperature superconductivity [1], [2]. Most of these ideas are centered around the notion that holes in metal oxide layers are described by an effective one-band Hubbard model resulting from integrating out degrees of freedom on the oxygen sites [3], or copper sites [4]. The bond between an oxygen atom and the two neighboring copper atoms is assumed to be a sigma bond in which the p_y ground state orbital on the oxygen atom atoms hybridizes strongly with both $d_{x^2-y^2}$ orbitals on the copper atoms. There has been much speculation as to the nature of the the ground state of this model, much of it involving novel physical and mathematical ideas [1], [2] in particular anyons [5]. Here a different starting point is suggested.

If the effect of oxygen nuclear motion is included, the p_y orbital becomes two states. Consider the situation depicted in fig.1abc. If the hole in this orbital is closer to one of the two copper atoms, say, atom A the oxygen atom will be pushed slightly towards or away from the other copper atom, called atom B . The sign of the pushing depends upon Coulombic as well as collective effects. It is assumed here that the overall consequence is that hybridization with the d orbital on atom A strengthens, while hybridization with the d orbital on atom B weakens. The effect of the local distortions of the lattice is that there is a double-well potential which must be added to the atomic potential in the Hamiltonian. The resulting Hubbard model has two sites instead of one associated with each oxygen atom. The ground state oxgen orbital is still p_y , but there is now an excited state whose wave function is symmetric along the x-axis.

It is important to stress that this proposal is not a B.C.S. picture. The lattice distortions have wavelengths the size of the interatomic spacing and do not give rise to long range forces by themselves. The mechanism of superconductivity is essentially magnetic.

A second assumption is also made; it is that the holes in the vicinity of a copper atom tend to form a spin singlet. The result is, after integrating out high frequency modes, an SU(2) lattice gauge theory, of the type studied in [6], [7]. The full gauge group is SU(2) \times U(1), including electromagnetism. The calculation is done perturbatively, much like that done for the one-band Hubbard model at half-filling to obtain the Heisenberg model (Mott-Hubbard insulator) [8]. These Hamiltonian lattice gauge theories, named gauge magnets in ref. [7], are rather different in structure from conventional lattice gauge theories. In particular, they are formulated in terms of only one representation of the gauge group. An SU(2) gauge transformation is the total spin in the vicinity of a copper atom; the two “colors” of the gauge theory are just \uparrow and \downarrow . This is closely related to the nondynamical gauge invariance noted by Baskaran and Anderson in the usual half-filled Hubbard model [9].

The effective gauge theory obtained has a superfluid, or Higgs field. It is in either the confined or the Higgs phase. General arguments [10] imply that that in either case the cell excitations are tightly paired into “baryon” excitations analogous to those in Q.C.D. Since the gauge group is SU(2) (instead of the SU(3) color group in Q.C.D.) these excitations are bound states of two cell excitations. The picture has some similarities with the U(1) gauge theory confinement schemes discussed by Wiegmann [2]

and Fradkin and Kivelson [11]. The Higgs field is (fractionally) charged, and so is a second (non-Cooper pair) carrier of supercurrent.

The situation on an oxygen atom is described (before considering hybridization) by the two-site Hamiltonian:

$$H = t_O \sum_{\alpha} c_{\vec{i},\alpha}^{\dagger} c_{\vec{j},\alpha} , \quad (1)$$

where \vec{i} , and \vec{j} are the different site locations, $\alpha = \uparrow, \downarrow$ and $c_{\vec{i},\alpha}^{\dagger}, c_{\vec{i},\alpha}$ are the creation and annihilation operators for holes. This Hamiltonian has a symmetric excited state lying at an energy twice the (wrong sign) oxygen hopping parameter, t_O , above the antisymmetric ground state.

A more precise statement of the second assumption is that, if one ignores the hopping between the two oxygen sites (1), then the ground state of the hole configuration on a copper site and the adjacent oxygen sites is a spin singlet, while the (spin degenerate) first excited state is not. The *cell* in the vicinity of the copper atom will be defined to be this set of sites. Spin non-singlets are excitations which can move from cell to cell through the lattice. The essential point of this paper is that they must move in a gauge covariant manner. The Gauss's law operator \vec{G} is the sum of two terms. The first term is the total spin \vec{S} in a particular cell. The second term is minus the sum over first excited states $|X\rangle$ of the excited state spin eigenvalue \vec{S}_X times the projection operator $|X\rangle\langle X|$ for that particular excited state. This Gauss's law operator will, by construction, obey the appropriate local commutation relations and annihilate physical states. By definition then Gauss's law is satisfied. Therefore SU(2) gauge invariance of the states is inevitable.

There are some possible objections that might be raised to the ideas presented here. The fact that motion of oxygen atoms is essential seems to suggest that a charged density wave would form. This is not true, as it is inconsistent with gauge invariance. Another objection might be that there are four states, rather than two on the oxygen orbitals. This is in fact so, but these states are not degenerate, and the ground state orbital is not significantly different from that indicated by experiments.

This article is a slightly revised version of a paper circulated in March, 1990, while the author was at Virginia Polytechnic Institute and State University.

2 Gauge Magnets

Lattice gauge magnets [6], [7] are gauge invariant generalizations of isotropic Heisenberg magnets. They are formulated quite differently from the usual Wilson or Kogut-Susskind lattice gauge theories. The first SU(2) gauge magnet Hamiltonian was written down by Horn [6] who proposed it as a simple regularization of Yang-Mills theory. The author and D. Rohrlich [7] showed that the Horn model has a nonrelativistic spin wave dispersion relation. It was also found that there is an enormous variety of SU(2) gauge magnets. Abelian gauge magnets have been studied as way of formulating short range resonating valence bond phases [11], [12]. For a more detailed discussion, see ref. [7].

In order to define gauge magnets for the spin-1/2 representation of SU(2), it is necessary to consider operators at the links of a square lattice, \vec{x}, \hat{m} connecting the

sites \vec{x} and $\vec{x} + a\hat{m}$, $m = 1, \dots, d$, where \vec{x} is a d -component site vector. The Hilbert space at each link is four-dimensional, so these operators can be thought of four-by-four matrices acting on a given link. These operators are Dirac matrices for a Euclidean metric, $\gamma^0(\vec{x}, m)$, $\gamma^1(\vec{x}, m)$, $\gamma^2(\vec{x}, m)$, $\gamma^3(\vec{x}, m)$, with the anticommutation relations

$$[\gamma^\mu(\vec{x}, m), \gamma^\nu(\vec{x}, m)]_+ = \delta^{\mu\nu}, \quad (2)$$

on the same link and the commutation relations

$$[\gamma^\mu(\vec{x}, m), \gamma^\nu(\vec{y}, n)] = 0, \quad (3)$$

on different links. It is important to emphasize that the greek indices μ, ν simply label different operators, and have nothing to do with space or time. The index m was called i in ref. [7]. A specific representation at one link is

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \vec{\gamma} = \begin{pmatrix} 0 & i\vec{\sigma} \\ -i\vec{\sigma} & 0 \end{pmatrix}, \quad (4)$$

where $\vec{\sigma}$ are the usual Pauli matrices. Other useful operators are

$$\gamma^5 = \gamma^0 \gamma^1 \gamma^2 \gamma^3, \quad \rho^\mu = -i\gamma^5 \gamma^\mu, \quad \sigma^{\mu\nu} = -\frac{i}{4}[\gamma^\mu, \gamma^\nu], \quad (5)$$

and

$$\Sigma^a = \frac{1}{2} \sum_{bc} \varepsilon^{abc} \sigma^{bc} - \sigma^{0a}, \quad \tilde{\Sigma}^a = \frac{1}{2} \sum_{bc} \varepsilon^{abc} \sigma^{bc} + \sigma^{0a}, \quad a, b, c = 1, 2, 3. \quad (6)$$

In the representation (4)

$$\vec{\Sigma} = \frac{1}{2} \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & 0 \end{pmatrix}, \quad \vec{\tilde{\Sigma}} = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & \vec{\sigma} \end{pmatrix}. \quad (7)$$

While the introduction of these operators may seem rather *ad hoc* at this stage, it will be shown in the next section that they can arise naturally in a particular Hubbard model of holes.

The basic lattice gauge fields are

$$U_{\alpha\beta}(\vec{x}, m) = \gamma^0 - i\vec{\gamma} \cdot \vec{x}, \quad (8)$$

and

$$U_{\alpha\beta}^5(\vec{x}, m) = \rho^0(\vec{x}, m) \delta_{\alpha\beta} - i\vec{\rho}(\vec{x}, m) \cdot \vec{\tau}_{\alpha\beta}. \quad (9)$$

Here the 2×2 matrices τ^1, τ^2, τ^3 are again the Pauli matrices. The gauge fields $U(\vec{x}, m)$ and $U^5(\vec{x}, m)$ should be thought of as operator valued 2×2 matrices; the indices α, β in (8) and (9) are simply labels of matrix rows and columns. The matrices τ^a do not act on the Hilbert space. The operators σ^a *do* act on the upper two components or lower two components of the Hilbert space, however.

The “vacuum” generators of gauge transformations are

$$\vec{G}(\vec{x}) = \sum_m [\vec{\Sigma}(\vec{x}, m) + \vec{\tilde{\Sigma}}(\vec{x} - a\hat{m}, m)] \quad (10)$$

and obey the local commutation relations

$$[G^a(\vec{x}), G^b(\vec{y})] = 2i \sum_c \varepsilon^{abc} \delta_{\vec{x}\vec{y}} G^c(\vec{x}). \quad (11)$$

The fields U, U^5 transform as “parallel transport” or “connection” fields: If $Y(\vec{x}, m)$ is any linear combination of $U(\vec{x}, m)$ and $U^5(\vec{x}, m)$ (with complex coefficients which can depend on the link) then :

$$[G^a(\vec{x}), Y(\vec{x}, m)] = -i\tau^a Y(\vec{x}, m), \quad [G^a(\vec{x}), Y(\vec{x} - a\hat{n}, m)] = iY(\vec{x}, m)\tau^a. \quad (12)$$

The right-hand-sides in (12) are matrix products over greek indices. It is simple to make gauge invariant quantities by multiplying U 's together, end to end. Some examples considered in ref. [7] were the gauge magnet Hamiltonians:

$$H = J \sum_{\vec{x}} \sum_{m \neq n} \text{Tr} U(\vec{x}, m) U(\vec{x} + \hat{m}, n) U(\vec{x} + \hat{n}, m)^\dagger U(\vec{x}, n)^\dagger, \quad (13)$$

(the trace is over greek indices) which has a nonrelativistic spin wave dispersion relation, and, in two spatial dimensions, the “staggered” model:

$$\begin{aligned} H &= J \sum_{x^1+x^2 \text{ even}} \text{Tr} U(\vec{x}, 1) U(\vec{x} + \hat{1}, 2) U(\vec{x} + \hat{2}, 1)^\dagger U(\vec{x}, 2)^\dagger, \\ &+ K \sum_{x^1+x^2 \text{ odd}} \text{Tr} U^5(\vec{x}, 1) U^5(\vec{x} + \hat{1}, 2) U^5(\vec{x} + \hat{2}, 1)^\dagger U^5(\vec{x}, 2)^\dagger, \end{aligned} \quad (14)$$

which has a relativistic massive dispersion relation, and was argued to be topologically massive SU(2) Yang-Mills theory [13] in ref. [7]. Another operator which commutes with all the G^a 's is $\gamma^5(\vec{x}, m)$, so this is also a possible term to include in a gauge magnet Hamiltonian.

Coupling a fermionic matter field $c_{\vec{x}, \alpha}$ to the gauge field

$$Y(\vec{x}, m) = r(\vec{x}, m) U(\vec{x}, m) + r^5(\vec{x}, m) U^5(\vec{x}, m) \quad (15)$$

is accomplished with

$$H_{eff}^1 = -T \sum_{\vec{x}, m} \sum_{\alpha, \beta} c_{\vec{x}, \alpha}^\dagger Y_{\alpha\beta}(\vec{x}, m) c_{\vec{x}, \beta} + h.c., \quad (16)$$

with the Gauss's law operator modified to

$$\vec{G}(\vec{x}) = \sum_m [\vec{\Sigma}(\vec{x}, m) + \vec{\Sigma}(\vec{x} - a\hat{m}, m)] + \frac{1}{2} \sum_{\alpha\beta} c_{\vec{x}, \alpha}^\dagger \vec{\tau}_{\alpha\beta} c_{\vec{x}, \alpha}. \quad (17)$$

3 The Hopping Parameter Expansion

A model Hubbard Hamiltonian with the features discussed in the introduction will now be studied in perturbation theory. It is somewhat unrealistic as the doping is far too large, and there is a hole for every oxygen atom. The basic idea should extend,

however, to the case of a more realistic doping concentration, as will be discussed at the end of this section. Perturbation theory is not quantitatively correct unless all hopping parameters are small. Nonetheless, it should be a good guide to the form of the effective Hamiltonian.

This two-dimensional Hubbard model describes the dynamics of holes hopping between sites \vec{i} on the lattice shown in fig.2. There are two available sites on each link (oxygen atom) and one available site at each intersection point (copper atom). Each copper atom together with the nearest neighbor sites on the adjacent oxygen atoms is regarded as a cell. Thus each cell has five sites. We can label the copper atoms by vectors $\vec{i} = \vec{x}$ and the sites on the oxygen atoms by $\vec{i} = \vec{x} \pm b\hat{m}$, where $m = 1, 2$ and $b < a/2$ is the spacing between a copper site and the nearest oxygen site. The cell containing \vec{x} and $\vec{x} \pm b\hat{m}$ will be denoted by $B_{\vec{x}}$. The sites in $B_{\vec{x}}$ can be written alternatively as $\vec{i} \in B_{\vec{x}}$. The oxygen atom connecting the sites \vec{x} and $\vec{x} + a\hat{m}$ will be denoted by $L_{\vec{x},\hat{m}}$. The sites on $\vec{x} + b\hat{m}$ and $\vec{x} + (a-b)\hat{m}$ can be written as $\vec{i} \in L_{\vec{x},\hat{m}}$. It is convenient to drop the subscripts from B and L .

The Hamiltonian has the form

$$H = H_0 + V. \quad (18)$$

The unperturbed part of (18) is:

$$\begin{aligned} H_0 = & U \sum_{\vec{x}} n_{\vec{x},\uparrow} n_{\vec{x},\downarrow} + J \sum_B \sum_{\vec{i} \neq \vec{j} \in B} \vec{S}_{\vec{i}} \cdot \vec{S}_{\vec{j}} + A \sum_{\vec{x}} (n_{\vec{x},\uparrow} + n_{\vec{x},\downarrow}) \\ & + D \sum_L \sum_{\vec{i} \neq \vec{j} \in L} (n_{\vec{i},\uparrow} + n_{\vec{i},\downarrow})(n_{\vec{j},\uparrow} + n_{\vec{j},\downarrow}) + \mu [\sum_i (n_{\vec{i},\uparrow} + n_{\vec{i},\downarrow}) - h]. \end{aligned} \quad (19)$$

The coefficients U , J , A and D are positive, and $U, D \gg J \gg A$. The first term of (19) is a repulsive interaction on copper atoms. The second term in (19) is an antiferromagnetic interaction between any two holes in the cell. The third term of (19) favors occupation of sites on the oxygen atoms over occupation of sites at the copper atoms. The fourth term in (19) discourages the occupation of any pair of sites on an oxygen atom by more than one hole. The last term enforces the hole number to be fixed to h .

Consider the situation in which the total number of holes, h in the model is set to be $2N$, where N is the total number of copper atoms. For large U , A and D the (highly degenerate) ground state of H_0 has two holes per cell, occupying two different links (fig.3). The configurations resemble those of two-dimensional cubic ice crystals (the six-vertex model). The lowest lying excited states can be made by taking a hole from one cell and placing it at the copper atom in another cell. The latter cell now contains a total of three holes, one hole at the copper atom and the remaining two hole on two different oxygen atoms. The energy of such states is of order J .

If the total number of holes is $(2 + \epsilon)N$ then a fraction ϵ of the cells will be excited. The lowest lying states will have holes at some copper atoms (fig.5). In these states, excited cells are the only cells which are not spin singlets. Their energy is of order ϵA .

The interaction of (18) introduces hopping between the sites:

$$V = - \sum_{\langle \vec{i}, \vec{j} \rangle} \sum_{\alpha} t_{\vec{i}, \vec{j}} c_{\vec{i}, \alpha}^{\dagger} c_{\vec{j}, \alpha}, \quad (20)$$

where the hopping parameters $t_{i,j}$ are regarded as small compared to the constants U, J, A and D . The hopping parameter between two sites on the same oxygen atom will be denoted by $t_{\vec{x}+b\hat{m}, \vec{x}+(a-b)\hat{m}} = -t_O$, as before, while that between copper and oxygen sites will be denoted by $t_{\vec{x}, \vec{x}\pm b\hat{m}} = t_{Cu-O}$.

This toy model now has the basic features discussed in the introduction. The lattice is broken up into cells, spin singlets are energetically favorable in the cells, and there is weak hopping between the cells. It will be verified in this section that, in the hopping parameter expansion, with the number of holes equal to $(2 + \epsilon)N$, this system is a gauge magnet. This expansion is not quantitatively correct, because in CuO_2 layers the parameter t_O must be actually bigger than A . In the limit that t_O becomes infinite, the system becomes a one-band Hubbard model [1]. What this means is that as t_O/A increases, there is eventually a transition to a phase described by the one-band model. Above this phase transition, the low frequency behaviour is that of the $t - J$ model [3]. It is a crucial assumption that t_O/A is fairly large (of one order of magnitude, say) at the phase transition. As long as t_O/A is below the transition point, the form of the resulting effective Hamiltonian obtained in perturbation theory will be correct. A pictorial comparison of the various constants in the model are shown in fig.5.

For $\epsilon \ll 1$ most of the excited cells (with a hole on the copper d orbital) will be surrounded by cells which are not excited. It is straightforward to see how an excitation moves through the lattice. Since A is the smallest of the constants in (18) the most significant energy denominator is $1/A$.

Consider the configurations of two adjacent cells in fig.6ab. The cell on the left is excited, while that on the right is not. The holes at sites other than the two copper atoms and the oxygen atom joining the cells are superfluous, so the configurations of fig.6a and fig.6b are conveniently labeled by the spin at these four sites, on a line from left to right:

$$|\uparrow, 0, \uparrow, 0\rangle, |\uparrow, 0, \downarrow, 0\rangle, |\downarrow, 0, \uparrow, 0\rangle, |\downarrow, 0, \downarrow, 0\rangle, \quad (21)$$

and

$$|\uparrow, \uparrow, 0, 0\rangle, |\uparrow, \downarrow, 0, 0\rangle, |\downarrow, \uparrow, 0, 0\rangle, |\downarrow, \downarrow, 0, 0\rangle, \quad (22)$$

respectively. The left-most spin is at \vec{x} , while the right-most spin is at $\vec{x} + a\hat{m}$.

The states (21) can undergo the following changes under hopping:

$$\begin{aligned} |\uparrow, 0, \uparrow, 0\rangle &\rightarrow |\uparrow, 0, 0, \uparrow\rangle \rightarrow |0, \uparrow, 0, \uparrow\rangle \\ |\uparrow, 0, \downarrow, 0\rangle &\rightarrow |\uparrow, 0, 0, \downarrow\rangle \rightarrow |0, \uparrow, 0, \downarrow\rangle \\ |\downarrow, 0, \uparrow, 0\rangle &\rightarrow |\downarrow, 0, 0, \uparrow\rangle \rightarrow |0, \downarrow, 0, \uparrow\rangle \\ |\downarrow, 0, \downarrow, 0\rangle &\rightarrow |\downarrow, 0, 0, \downarrow\rangle \rightarrow |0, \downarrow, 0, \downarrow\rangle \end{aligned} \quad (23)$$

The intermediate states are short lived; the lifetime is of order \hbar/A . The matrix elements of the Hamiltonian between the initial and final states of (23) are to second order in perturbation theory given by

$$\begin{aligned} \langle \uparrow, 0, \uparrow, 0 | H | 0, \uparrow, 0, \uparrow \rangle &= \langle \uparrow, 0, \uparrow, 0 | H | 0, \uparrow, 0, \uparrow \rangle = \langle \uparrow, 0, \uparrow, 0 | H | 0, \uparrow, 0, \uparrow \rangle \\ &= \langle \uparrow, 0, \uparrow, 0 | H | 0, \uparrow, 0, \uparrow \rangle = -t_{Cu-O}^2/A. \end{aligned} \quad (24)$$

It is now possible to write an effective Hamiltonian for the low lying states; these do not include the intermediate states of (24). This amounts to integrating out modes of frequency A/\hbar , while ignoring modes of higher frequency. Consider the operators $Y^0(\vec{x}, m), \vec{Y}(\vec{x}, m)$ acting only on the spins of the oxygen atom by

$$\begin{aligned} Y^0(\vec{x}, m) &= \sum_{\alpha} c_{\vec{x}+b\hat{m},\alpha}^{\dagger} c_{\vec{x}+(a-b)\hat{m},\alpha} , \\ Y^1(\vec{x}, m) &= i \sum_{\alpha} c_{\vec{x}+b\hat{m},\alpha}^{\dagger} c_{\vec{x}+(a-b)\hat{m},-\alpha} , \\ Y^2(\vec{x}, m) &= - \sum_{\alpha} \text{sgn}(\alpha) c_{\vec{x}+b\hat{m},\alpha}^{\dagger} c_{\vec{x}+(a-b)\hat{m},-\alpha} , \\ Y^3(\vec{x}, m) &= i \sum_{\alpha} \text{sgn}(\alpha) c_{\vec{x}+b\hat{m},\alpha}^{\dagger} c_{\vec{x}+(a-b)\hat{m},\alpha} , \end{aligned} \quad (25)$$

with the conventions $\text{sgn}(\uparrow) = 1, \text{sgn}(\downarrow) = -1$ and $-\uparrow = \downarrow$. The low energy, effective Hilbert space on an oxygen atom is four-dimensional. On this Hilbert space it is easy to see that under the identification

$$\begin{aligned} |\cdot, \uparrow, 0, \cdot\rangle &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} , \quad |\cdot, \downarrow, 0, \cdot\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} , \\ |\cdot, 0, \uparrow, \cdot\rangle &= \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} , \quad |\cdot, 0, \downarrow, \cdot\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} , \end{aligned} \quad (26)$$

one finds, in the notation of the previous section,

$$Y^{\mu}(\vec{x}, m) = \frac{\gamma^{\mu}(\vec{x}, m) + i\rho^{\mu}(\vec{x}, m)}{2} . \quad (27)$$

The lattice gauge field is

$$\begin{aligned} Y_{\alpha\beta}(\vec{x}, m) &= Y^0(\vec{x}, m) \delta_{\alpha\beta} - i\vec{Y}(\vec{x}, m) \cdot \vec{\tau}_{\alpha\beta} \\ &= \frac{1}{2} U_{\alpha\beta}(\vec{x}, m) + \frac{i}{2} U_{\alpha\beta}^5(\vec{x}, m) \end{aligned} \quad (28)$$

The effective Hamiltonian has a term generated by the process (23)

$$H_{eff}^1 = -\frac{t_{Cu-O}^2}{A} \sum_{\vec{x}, m} \sum_{\alpha, \beta} c_{\vec{x}, \alpha}^{\dagger} Y_{\alpha, \beta}(\vec{x}, m) c_{\vec{x}+a\hat{m}, \beta} + h.c., \quad (29)$$

which is an SU(2) gauge invariant hopping term.

The processes of cell excitation transport involving states (22) have not yet been considered. The processes involving these states have (21) as intermediate states. They are therefore included in the effective Hamiltonian by introducing a term connecting $|\cdot, \alpha, 0, \cdot\rangle$ and $|\cdot, 0, \alpha, \cdot\rangle$. This term can be read off from (1) and (26) :

$$H_{eff}^2 = t_O \sum_{\vec{x}, m} \gamma^0(\vec{x}, m) . \quad (30)$$

It breaks the SU(2) gauge invariance explicitly, by giving some of the gauge spin waves a gap.

The operator (17) is the same as

$$\vec{G}(\vec{x}) = \frac{1}{2} \sum_{\vec{i} \in B_{\vec{x}}} \sum_{\alpha\beta} c_{i,\alpha}^\dagger \vec{\tau}_{\alpha\beta} c_{i,\beta}, \quad (31)$$

which is just the total spin in a cell. The “color” of the SU(2) gauge theory is simply spin. This operator commutes with (29), but not (30).

Equation (30) can also be viewed as the gauge invariant Hamiltonian for an additional spin-zero field coupled to Y . The term

$$H_{eff}^2 = t_O \sum_{\vec{x}, m} \sum_{\alpha\beta\gamma} \phi_{\alpha\beta}^\dagger(\vec{x}) Y_{\beta\gamma}(\vec{x}, m) \phi_{\gamma\alpha}(\vec{x} + a\hat{m}) + h.c., \quad (32)$$

where $\phi(\vec{x})$ is a unitary (c-number) 2×2 matrix, $\phi^\dagger(\vec{x})\phi(\vec{x}) = 1$, provided the Gauss’ law operator is modified to

$$\begin{aligned} \vec{G}(\vec{x}) = & \sum_m [\vec{\Sigma}(\vec{x}, m) + \vec{\Sigma}(\vec{x} - a\hat{m}, m)] + \frac{1}{2} \sum_{\alpha\beta} c_{\vec{x},\alpha}^\dagger \vec{\tau}_{\alpha\beta} c_{\vec{x},\alpha} \\ & + \frac{1}{2} \sum_{\alpha\beta\gamma} \vec{\tau}_{\alpha\beta} \phi_{\beta\gamma}(\vec{x}) \frac{\partial}{\partial \phi_{\gamma\alpha}(\vec{x})} - \frac{1}{2} \sum_{\alpha\beta\gamma} \phi_{\alpha\beta}^\dagger(\vec{x}) \vec{\tau}_{\beta\gamma} \frac{\partial}{\partial \phi_{\gamma\alpha}^\dagger(\vec{x})}, \end{aligned} \quad (33)$$

reduces to (30) in a particular gauge (known as the “unitary gauge”) in which $\phi_{\alpha\beta}(\vec{x}) = \delta_{\alpha\beta}$. The field ϕ describes a chiral spin superfluid.

When the effect of electromagnetism is included the Hamiltonian must be modified. Taking $A_0 = 0$ gauge, (29) and (32) become, respectively :

$$H_{eff}^1 = -\frac{t_{Cu-O}^2}{A} \sum_{\vec{x}, m} \sum_{\alpha,\beta} c_{\vec{x},\alpha}^\dagger Y_{\alpha\beta}(\vec{x}, m) \exp \left[ie \int_{\vec{x}}^{\vec{x}+a\vec{m}} A_m dx^m \right] c_{\vec{x}+a\vec{m},\beta} + h.c., \quad (34)$$

and

$$\begin{aligned} H_{eff}^2 = & t_O \sum_{\vec{x}, m} \sum_{\alpha\beta\gamma} \phi_{\alpha\beta}^\dagger(\vec{x}) Y_{\beta\gamma}(\vec{x}, m) \\ & \times \exp \left[i \left(1 - \frac{2b}{a} \right) e \int_{\vec{x}}^{\vec{x}+a\vec{m}} A_m dx^m \right] \phi_{\gamma\alpha}(\vec{x} + a\hat{m}) + h.c.. \end{aligned} \quad (35)$$

In (35) the approximation was made that the vector potential \vec{A} is smoothly varying (in the exact expression, the range of integration in the Aharonov-Bohm phase factor is from $\vec{x} + b\vec{m}$ to $\vec{x} + (a - b)\vec{m}$). The superfluid field has fractional charge $(1 - 2b/a) e$. Even without proceeding further, it is clear that this field already produces superconductivity. Cooper pairing of cell excitations also occurs, making a total of two superfluid condensates.

Thus far the part of the Hamiltonian depending only on the gauge field has been ignored. Such a term will be generated by higher orders in the hopping parameter expansion. The leading contribution is a plaquette interaction

$$H_{eff}^3 = (t_{Cu-O}/A)^4 \sum_{\vec{x}} \sum_{m \neq n} \text{Tr} Y(\vec{x}, m) Y(\vec{x} + \hat{m}, n) Y(\vec{x} + \hat{n}, m)^\dagger Y(\vec{x}, n)^\dagger + h.c. . \quad (36)$$

If high frequency Fourier components of $c_{\vec{x},\alpha}$, $c_{\vec{x},\alpha}^\dagger$ are integrated out, there is an additional contribution of the form (36). The spin wave spectrum of (36) will be studied elsewhere. The coefficient of this term is extremely small in this perturbative analysis; but this analysis is only meant to be a guide to obtaining H_{eff} . If t_{Cu-O} is larger than A , there is no reason to expect this term to be small. In two space and one time dimension, a dynamical non-Abelian gauge field coupled to a Higgs field will either confine or screen the sources (which are holes at copper sites).

Holes in real high-temperature superconductors have a much lower concentration than in this toy model. Only a small number of oxygen atoms are actually doped, i.e. $2N \gg h$. The remaining oxygen sites are not occupied by holes in low-lying states. The system is described by the unextended Hubbard model on the lattice of fig.2:

$$H = - \sum_{\langle \vec{i}, \vec{j} \rangle} \sum_{\alpha} t_{\vec{i}, \vec{j}} c_{\vec{i}, \alpha}^\dagger c_{\vec{j}, \alpha} + \sum_{\vec{i}} U_{\vec{i}} n_{\vec{i}, \uparrow} n_{\vec{i}, \downarrow} + \mu [\sum_i (n_{i, \uparrow} + n_{i, \downarrow}) - h] . \quad (37)$$

Again there are two hopping parameters, $t_{\vec{x}+b\hat{m}, \vec{x}+(a-b)\hat{m}} = -t_O$, $t_{\vec{x}, \vec{x} \pm b\hat{m}} = t_{Cu-O}$. There are two coulomb repulsion strengths, $U_{\vec{x}} = U_{Cu}$ on copper sites and $U_{\vec{x} \pm b\hat{m}} = U_O$ on oxygen sites. The issue is now whether the model (18) is a good description of the physics at distances of two or three lattice spacings. I conjecture that undoped regions of a few lattice spacings in diameter behave as cells connected by doped oxygen bonds, and that (18) arises as a real space renormalization of (37)

4 Confinement and Higgs Phases

Ignoring the Higgs field ϕ , the system will be in the confined phase. That means that holes at the copper sites are confined into spin-singlet pairs. Separating a pair sufficiently far leads to the formation of a “spino-electric” string between them. This string is a line of non-Abelian electric flux. Its energy is proportional to its length (there is a string tension). An operator which creates such a hole-string-hole excitation on the ground state is

$$\beta(x, y; C) = c^\dagger(\vec{x}) \prod_{l \in C} Y(l) \tau^2 c^\dagger(\vec{z}) , \quad (38)$$

where l is a link along the path C between the holes at the copper sites \vec{x} and \vec{z} . This is an SU(2) baryon creation operator. It is a bound state of two cell excitations. A neutral meson-type excitation produced by

$$\mu(x, y; C) = c^\dagger(\vec{x}) \prod_{l \in C} Y(l) d^\dagger(\vec{z}) , \quad (39)$$

where $d^\dagger(\vec{z})$ creates an electron at a copper site, can also exist, though it will have a much greater gap (because a single electron on the copper atom has a very large energy). There are also anti-baryon states containing two electrons. The string can break only if new holes or electrons appear on copper sites, to join to the new string ends. These particles must be pulled out of the Fermi sea, at a large cost in energy

(because if the string breaks, it is inevitable that at least one electron is produced at a copper site). Thus, unlike the situation in Q.C.D., fragmentation of strings is rare. It is operators such as β which will condense in the ground state, leading to superconductivity.

Now suppose the Higgs field is coupled into the system. This field is a unitary matrix which transforms according to the fundamental representation of $SU(2)$. It breaks the effective gauge symmetry completely. Nonetheless a confined phase is still conceivable. There are in fact two possible phases for an $SU(N)$ gauge theory in two space and one time dimension. The other phase, in which the Higgs field screens adjoint sources, is called the Higgs phase [14]. This phase also has a gap. Fradkin and Shenker [10] showed that in this situation, the phases are one and the same. In the Euclidean lattice formulation, the phase boundary terminates in a critical point, beyond which the phases are connected. The physical reason is that the basic excitations in the confined phase and the Higgs phase can be made by acting with the same operators on the ground state. A pair of holes is no longer bound by a string, but is instead screened by Higgs quasiparticles. The operator which makes these quasiparticles on the ground state is, in the unitary gauge, the same operator which created the spino-electric string in the confined phase. Therefore pairing and superconductivity will still occur. The size of the pair will now be determined by the screening length instead of the string tension.

5 Conclusions

By including the effect of local lattice distortions in CuO_2 layers, a new kind of Hubbard model has been proposed, with two sites on the links of the lattice. By integrating out high frequency modes in strong coupling perturbation theory a lattice gauge magnet was obtained. The resulting theory confines or screens the spin of hole quasiparticles at the intersection points (copper atoms), resulting in pairing and superconductivity. Because of the role of oxygen nuclear motion, at least a weak oxygen isotope effect should result. There is an second charge condensate, corresponding to the Goldstone mode of the fractionally charged, spinning Higgs field.

This theory of superconductivity has an appealing feature. It is an attempt to describe the physics at all relevant wavelengths, from the interatomic spacing to the macroscopic effective Hamiltonian. Most of the field theoretic ideas are in accord with long prevailing conventional wisdom.

Although perturbation theory was used to obtain this result, it is only good quantitatively for very small hopping parameters t_{Cu-O}, t_O . Even though t_O is much larger than the energy scale A , a gauge theory of the sort derived here should still describe the effective low frequency dynamics, provided t_O/A is below a certain critical value. At this value there is a phase transition to the $t - J$ model.

The mechanism proposed is not fundamentally two-dimensional. Three-dimensional Hubbard models can also be described by non-Abelian gauge theories. In three dimensions we expect that the phase transition, to a phase in which the holes are unbound, occurs at a lower value of T_c . Perhaps three-dimensional superconducting

bismuth oxide materials such as $Ba_{1-x}Pb_xBi_xO_3$ and $Ba_{1-x}K_xBiO_{3-y}$ [15] are also described by the picture presented here.

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7 Figure Captions

- Figure 1:
 - a) Oxygen displacement for a hole in the oxygen orbital near copper atom A. In this example the oxygen atom is attracted by the hole.
 - b) Oxygen displacement for a hole in the oxygen orbital near copper atom B.
 - c) Effective double well potential.
- Figure 2: The lattice of the Hubbard model. The dotted lines enclose a cell.
- Figure 3: A low-lying configuration of holes for hole number equal to $2N$. Note that the hole positions resemble those of hydrogen ions in two-dimensional ice models.
- Figure 4: A low-lying configuration of holes for hole number slightly greater than $2N$. Excited cells are shaded.
- Figure 5: The energy parameters $A, t_{Cu-O}, -t_O$. On the left side of the figure, t_O is in the regime where the hopping parameter expansion is valid. This parameter increases from the left to the right side of the figure. Eventually there is a phase transition to where the physics is described by the $t - J$ model.
- Figure 6:
 - a) An excitation in the cell at the left.
 - b) Another example of such an excitation.

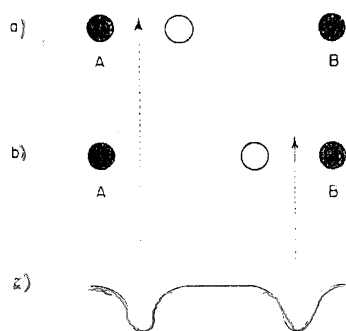


Fig. 1

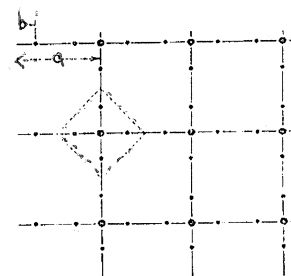


Fig. 2

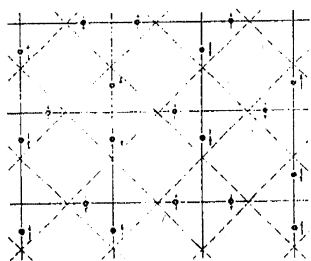


Fig. 3

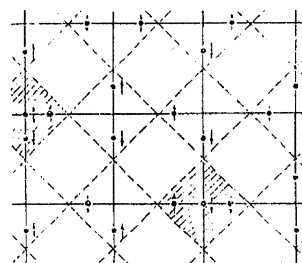


Fig. 4

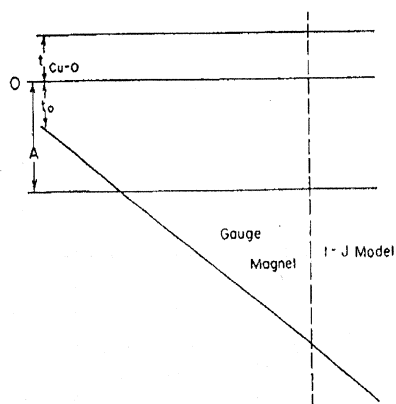


Fig. 5

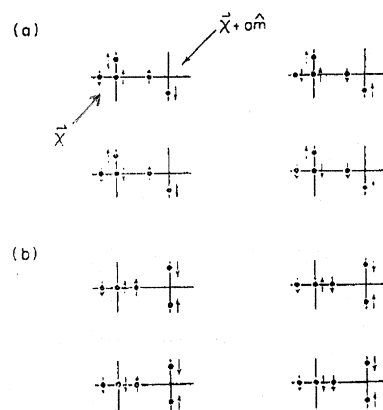


Fig. 6